Electronic Supplementary Material (ESI) for Environmental Science: Nano.

The adsorption and oxidation of SO_2 on MgO surface: Experimental and DFT calculation studies

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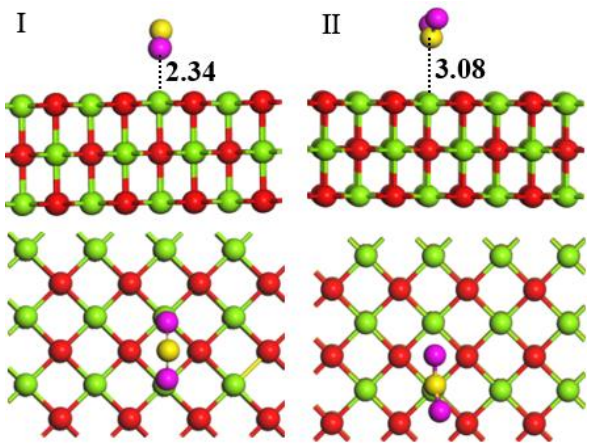

Fig. S1 Another two optimized configurations of SO_2 on perfect MgO(00) surface

Table S1. The IR vibrational frequencies and adsorption energies of adsorbed SO_2 at the MgO (001) surface (frequencies in cm^{-1}, adsorption energies in eV).

	Modes	**I**	**II**	**III**	**SO_2**
SO_2 frequency	δ	553	484	493	492
	ν_s	988	991	1077	1089
	ν_{as}	1056	1201	1270	1277
S-O bond length (Å)		1.47	1.45	1.44	1.43
Adsorption Energy (eV)		-1.03	-0.31	-0.20	—

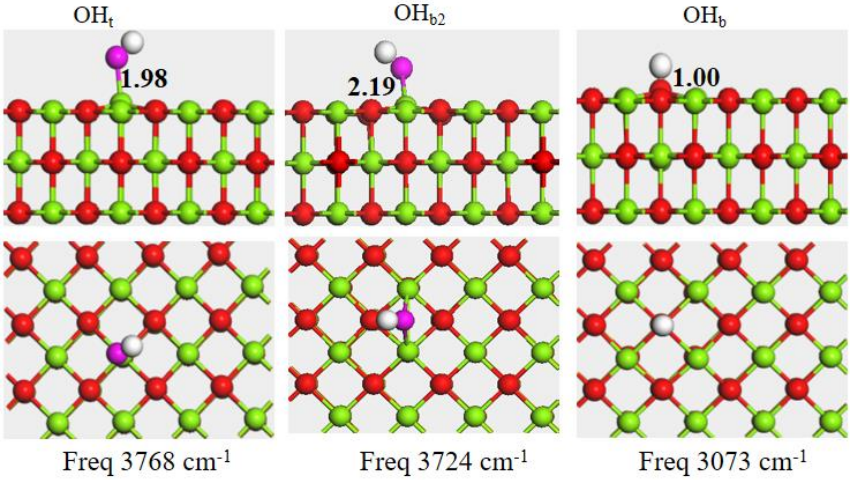

Fig. S2 The optimized structures of surface OH on MgO(100) surface

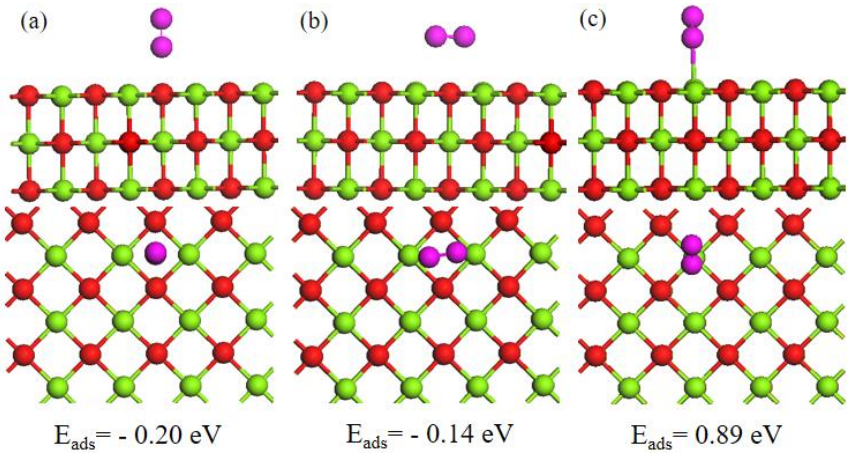

Fig. S3 The optimized structures and corresponding adsorption energies of O_2 adsorption on MgO(100) surface

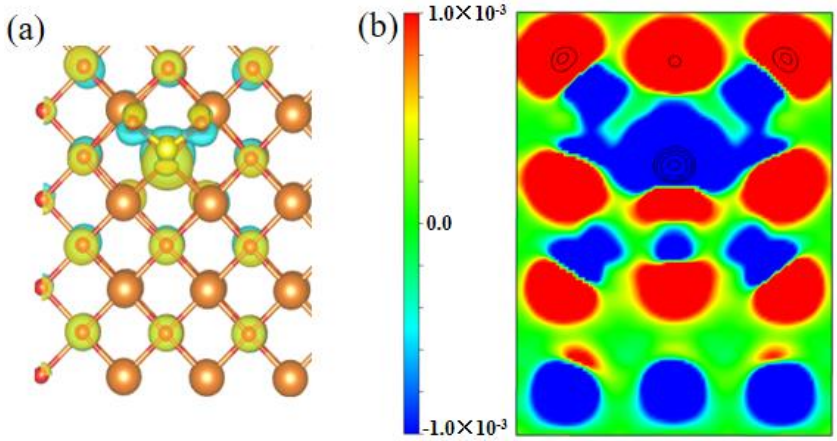

Fig. S4 Charge Density Difference (CDD) of SO_2 on a plane of MgO surface (a) 3D, the yellow and blue represent the increasment and decrement of electron density, respectively (b) 2D plot of CDD on MgO(001) surface, unit is e/bohr^3.

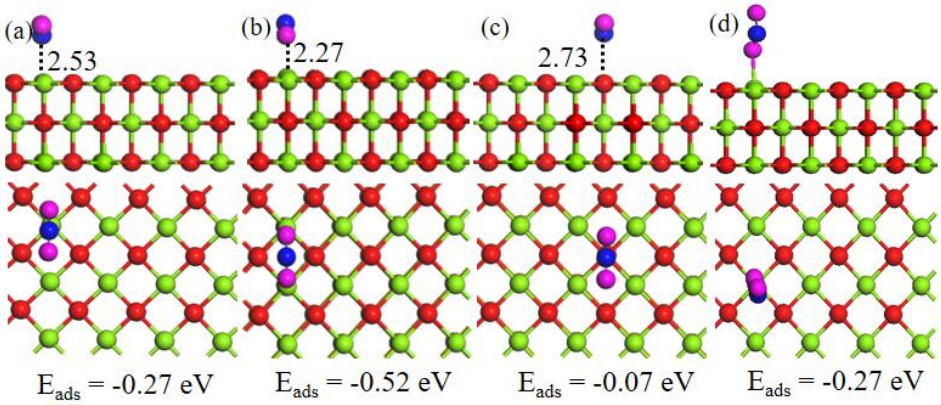

Fig. S5 The optimized adsorption configurations of NO_2 on MgO(100) surface

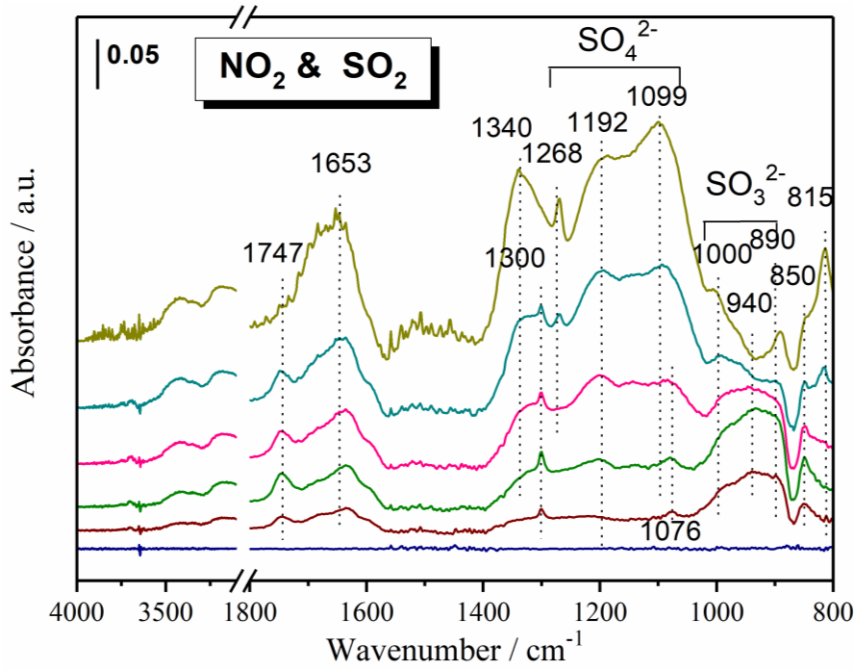

Fig. S6 Dynamic changes in the *in situ* DRIFTS spectra of the CaO sample as a function of time with a flow of 200 ppmv SO_2 + 200 ppmv NO_2 + 20% O_2 + 80% N_2 at 303 K. Total flow rate was 100 mL·min^{-1}.